

SAT Report for Case # P-18-0077

General

Report Status:	Complete	Status Date:	01/03/2018
CRSS Date:	01/04/2018	SAT Date:	01/05/2018
Consolidated PMN?		SAT Chair:	T. Behrsing
Consolidated Set:			
Submitter:	Koch		
	Agronomic Services		
CAS Number:	2093385-47-6		
Ecotox Analogs:			
Related Cases:			
Health Related Cases:	ANALOGS:		
Chemical Name:	Urea, reaction products with N-butylphosphorothioic triamide and formaldehyde		
Use:	Reagent for the controlled release of a urease inhibitor in urea-based fertilizers used on farms. %Phosphorus = 12.4% (measured). P2REC: CRSS: Forward. P2 Claim: The PMN material is intended to replace direct use of N-butyl-phosphorothioic triamide () in fertilizer formulations. NBPT, when in contact with the soil, degrades in a relatively short period of time through oxidation and hydrolysis. The PMN material is stable enough to extend the availability of NBPT, while being labile enough that NBPT is released when water is present, ensuring that a low level of NBPT is present for the days or weeks during which the urea fertilizer is taken up by the crop.		
Trade name:	Anvol (TM)-trademarked name of the final product formulation		
PV Max (kg/yr):			
Ecotox Assessor:	Amuel Kennedy	Fate Assessor:	Marcy Card
		Health Assessor:	A. Babcock

Physical Chemical Information

Molecular Weight:	239.23	Physical State - Neat:	Solid
Percent 500:		Percent 1000:	
Melting Point (Measured):		Melting Point (est):	Dec. ca. 150
Vapor Pressure:		Vapor Pressure (est):	0.000003
Water Solubility:	0.035000	Water Solubility (EST):	37.1/ [REDACTED]
Log Kow:		Log P Comment:	
		MPD (EPI):	
		VP (EPI):	
		Water Solubility (EPI):	
		Log Kow (EPI):	

SAT Concern

Ecotox Rating (1):	2	Ecotox Rating Comment (1):	
Ecotox Rating (2):		Ecotox Rating Comment (2):	
Health Rating (1):	2	Health Rating Comment (1):	
Health Rating (2):		Health Rating Comment (2):	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
1	1	2	PMN
3	1	2	Hyd Pdt NBPT

Persistence	Bioaccumulation	Toxicity	Comments
1	1	2	Hyd Pdt urea-formaldehyde oligomers

Exposure Based Review (Health)? Y
Exposure Based Review (Ecotox)? Y
SAT IRR, SENS, NEURO, REPRO,
Keywords: KIDNEY

Fate Assessment P-18-0077

Summary: FATE: Estimations for hydrolysis
 product N-butylphosphorothioic triamide,
 MW = 167, C₄H₁₄N₃PS
 log
 Kow = 0.44 (M)
 log Koc = 1.34 (E)
 log Fish BCF = 0.50 (3) (E)

 log Fish BAF = 0.03 (1) (E)
 FATE: Estimations for hydrolysis
 product urea-formaldehyde oligomer, MW = 162, C₄H₁₀N₄O₃
 log Kow = -4.01
 (E)
 log Koc = 1.00 (E)
 log Fish BCF = 0.50 (3) (E)
 log Fish
 BAF = -0.05 (1) (E)
 PMN Substance: Solid with MP = Dec. 150 °C (M)

 log Kow = 0.60 (M for mixture)
 S = Reacts / 35 mg/L at 25 °C / 37
 g/L at 25 °C (M / M for mixture / E)
 Hydrolysis Half-life = hr-da

 VP = 3.3E-6 torr at 25 °C (E)
 BP = 393 °C (E)
 H < 1.00E-8
 (E)
 POTW removal (%) = PMN 90 via hydrolysis; then Hyd Pdt NBPT 0-10;

 Hyd Pdt urea-formaldehyde oligomers 75-90 via biodeg and hydrolysis;

Hydrolysis (OPPTS 835.2120): $t_{1/2}(pH4,7,9)$:hr/hr-da/da
 Time for
 complete ultimate aerobic biodeg = Hyd Pdt NBPT > mo;
 Hyd Pdt
 urea-formaldehyde oligomers wk
 Sorption to soils/sediments = Hyd Pdt
 NBPT low; Hyd Pdt urea-formaldehyde oligomers low
 PBT Potential: PMN
 P1B1; Hyd Pdt NBPT P3B1; Hyd Pdt urea-formaldehyde oligomers P1B1
 *CEB
 FATE: Migration to ground water = Hyd Pdt NBPT rapid;
 Hyd Pdt
 urea-formaldehyde oligomers slow
 Bioconcentration factor to be put
 into E-FAST: Hyd Pdt NBPT 3;
 Hyd Pdt urea-formaldehyde oligomers 3

PMN Material:

Overall wastewater treatment removal is 90% via
 rapid hydrolysis (hydrolysis half-life: hours to days).

PMN

Material:

Low Persistence (P1) is based on rapid hydrolysis
 (hydrolysis half-life: hours to days).

Low Bioaccumulation potential

(B1) is based on rapid hydrolysis (hydrolysis half-life: hours to days).

Hydrolysis Product (N-butylphosphorothioic triamide):

Overall

wastewater treatment removal is 0-10% via low biodegradability, low
 sorption and low stripping.

Sorption to sludge is low based on the
 estimated physical-chemical properties from EPISUITE and STPWIN model
 estimates.

Air Stripping (Volatilization to air) is negligible based
 on the estimated physical-chemical properties from EPISUITE and STPWIN
 model estimates.

Removal by biodegradation in wastewater treatment
 is negligible based on BIOWIN model estimates and data from analogous
 chemicals.

The aerobic aquatic biodegradation half-life is greater
 than months based on BIOWIN model estimates and data from analogous
 chemicals.

The anaerobic aquatic biodegradation half-life is greater
 than months based on the aerobic biodegradation half-life. The anaerobic

biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.

Hydrolysis half-life is greater than months based on measured data (hydrolysis half-life: 92 days at pH 7 and 58 minutes at pH 3).

Sorption to soil and sediment is low based on the estimated physical-chemical properties from EPISUITE.

Migration to groundwater is rapid based on the estimated physical-chemical properties from EPISUITE.

Hydrolysis Product

(N-butylphosphorothioic triamide):

High Persistence (P3) is based on the estimated anaerobic biodegradation half-life.

Low

Bioaccumulation potential (B1) is based on the BCFBAF model estimates.

Hydrolysis Product (Urea-Formaldehyde oligomer):

Overall

wastewater treatment removal is 75-90% via biodegradation and hydrolysis.

Sorption to sludge is low based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.

Air Stripping

(Volatilization to air) is negligible based on the estimated physical-chemical properties from EPISUITE and STPWIN model estimates.

Removal by biodegradation in wastewater treatment is moderate based on BIOWIN model estimates.

The aerobic aquatic biodegradation half-life is weeks based on BIOWIN model estimates.

The anaerobic aquatic biodegradation half-life is greater than months based on the aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.

Hydrolysis half-life is days based on analogous chemicals and professional judgment.

Sorption to soil and sediment is low based on the estimated physical-chemical properties from EPISUITE.

Migration to groundwater is slow, mitigated by biodegradation and hydrolysis.

Hydrolysis Product (Urea-Formaldehyde oligomer):

Low Persistence (P1) is based on further hydrolysis of the urea-formaldehyde oligomer (hydrolysis half-life: days).

Low

Bioaccumulation potential (B1) is based on BCFBAF model estimates.

Bioconcentration/Bioaccumulation factor to be put into E-Fast: 3 (hydrolysis products).

Removal in 90;0-10;75-90
WWT/POTW
(Overall):

Condition	Rating Values w/ Rating Description	Comment
WWT/POTW	;1;1	
Sorption:		
WWT/POTW	;4;4	
Stripping:		
Biodegradation	;4;3	
Removal:		
Biodegradation		
Destruction:		
Aerobic Biodeg	;4;2	
Ult:		
Aerobic		
Biodeg Prim:		
Anaerobic Biodeg	;4;4	
Ult:		
Anaerobic		
Biodeg Prim:		
Hydrolysis (t1/2 at pH 7,25C) A:	2-3	P-NR
Hydrolysis (t1/2 at pH 7,25C) B:		
Sorption to	;4;4	
Soils/Sediments:		
Migration to	;4;2	
Ground Water:		;Hyd Pdt NBPT rapid; Hyd Pdt XXXXXXXXXX oligomers slow
Photolysis A,		
Direct:		

Condition	Rating Values w/ Rating Description	Comment
Photolysis B, Indirect: Atmospheric Ox A, OH: Atmospheric Ox B, O3:		

Health Assessment

Health Summary: Absorption is nil through the skin as the neat material and poor through the skin when in solution based on analog (a dermal absorption rate = 1 - 5% was used in the risk assessment for [REDACTED]). Expect good absorption through the lungs and GI tract based on physical/chemical properties. A 28-day study on the PMN suggests reduced erythrocyte (RBC) and brain cholinesterase activity but study error prevented a NOAEL determination. Data for N-(butyl)thiophosphoric triamide (NBPT; [REDACTED]) a component of the PMN and a degradation product of other components of the PMN, suggest concerns for dermal irritation (as observed in the acute dermal toxicity test), neurotoxicity, reproductive toxicity, kidney toxicity and sensitization. Repeated dose studies on the analog suggest 17.4 mg/kg as a LOAEL. Based on discussion at SAT, concerns for carcinogenicity from inhalation of formaldehyde degradation products is limited/unexpected due to the slow potential release. Release may be greater in acidic environmental conditions.

Routes of Exposure: Dermal Drinking Water
Exposure: Inhalation

Test Data Submitted

Test Data Submitted:

Test Data Submitted with the PMN:

- Acute oral toxicity study (up-and-down procedure in female rats)– LD50>2000 mg/kg; clinical signs limited to transient reduced fecal volume and soft feces
- Repeated dose 28-day oral gavage study in rats (250, 500, and 1000 mg/kg/day) - NOAEL for systemic effects was reported to be 1000 mg/kg/day; Erythrocyte (RBC) and brain cholinesterase activities were reduced in the high dose group. Because blood and brain tissue samples were discarded,

cholinesterase activities could not be determined for the mid- and low-dose groups, and thus no NOAEL can be determined for the cholinesterase inhibition effect. (also submitted as [REDACTED])

Analog data submitted under [REDACTED] as reported in [REDACTED] (same as [REDACTED]) SAT Report:

- Negative in Ames assay
- Negative in mouse micronucleus assay, ip
- Negative in CHO/HGPRT forward mutation assay
- Rat acute oral LD50 > 4.2 g/kg, possible signs of neurotoxicity noted
- Rat acute oral LD50 is 1 to 4 g/kg, NOEL = 300 mg/kg, signs of neurotoxicity, effects on heart and spleen
- Rabbit dermal LD50 > 2 g/kg with irritation at site of application
- Rat acute ocular study - no effect
- In vitro colorimetric assay for cholinesterase inhibition - no inhibition at mg %
- Mild dermal sensitizer in guinea pigs
- Absorption/metabolism study - readily absorbed via the GI tract and readily metabolized; excreted in 168 hours mostly in the form of urea or carbon dioxide
- 2-week range-finding oral study in rats - decreased body weight and blood urea nitrogen (BUN); cholinesterase; interpreted by EPA as an indication of neurotoxicity [REDACTED]
- 15-day oral study in rats - NOEL = 250 mg/kg but no histopathological examination was conducted (may be the same study as submitted under [REDACTED])
- 90-day dietary study in rats - LOAEL = 200 ppm in females (17.4 mg/kg) - fluid distension of the uterus, luminal dilatation of the uterus; reduced body weight gain and increased liver and uterine weights at higher doses; neurotoxicity component of this study showed a transitory decrease in grip strength at 5 weeks in the high dose group (5000 ppm)
- 2-generation reproductive effects study in rats - NOEL for reproductive effects is 800 ppm in females (61 mg/kg) and 200 ppm for males based on epididymal lesions and decreased sperm motility
- Oral developmental toxicity study in rats NOEL = 500 mg/kg (highest dose

tested) for fetotoxicity; maternal NOEL is between 30 and 125 mg/kg based on salivation, decreased weight gain, and noisy respiration

- Oral

developmental toxicity study in rabbits - NOEL = 200 mg/kg (highest dose) for fetotoxicity; maternal NOEL = 50 mg/kg based on subcapsular scarring of the kidneys

- Developmental toxicity study in mice - no other information available; notation in 5(e) test database, but no summary or review of study readily available

Ecotox Assessment

Test organism	Test Type	Test Endpoint	Predicted	Measured	Comments
Fish	96-h	LC50	>100	780	Est Top Left; Anlg [REDACTED]
Daphnid	48-h	LC50	>100	290	" "
Green Algae	96-h	EC50	8.4	280	" "
Fish	-	Chronic Value	>10	78	Est Top Left; Anlg [REDACTED] ACR10
Daphnid	-	Chronic Value	>10	29	Est Top Left; Anlg [REDACTED] ACR10
Green Algae	-	Chronic Value	2.8	97	" "

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute		4	2100	Algae
Chronic		10	280	Algae

Ecotox Route of Exposure? All releases to water

Factors	Values	Comments
SARs:	Substituted Ureas	
SAR Class:	Substituted Ureas- Thiophosphoramidate	
TSCA	None	
NCC Category?		

Recommended Testing

Ecotox Value Comments

Predictions are based on QSARs for substituted ureas (ECOSAR V2.0); MW 239; Log Kow = 0.60 (M, for mixture); solid with an unknown MP (P); S = 35 mg/L (M, for mixture), Reacts; effective concentrations based on 100% active

ingredients and mean measured concentrations; hardness <150 mg/L as CaCO₃; and TOC <2.0 mg/L.

Ecotox Factors

Comments

Environmental Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (<https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model>).

Based on these estimated hazard values from ECOSAR, EPA concludes that this chemical substance has moderate environmental hazard.

- Substance does not fall within the TSCA New Chemicals Categories.
- ECOSAR chemical class of Substituted Ureas.
- Analog data were considered for [REDACTED]
- .

Moderate hazard based on acute and chronic concentrations of concerns

of 2,100 ppb and 280 ppb, respectively.